Comment on "Equivalence of the variational matrix product method and the density matrix renormalization group applied to spin chains" by J. Dukelsky, M. A. Martín-Delgado, T. Nishino and G. Sierra

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Dukelsky, Martín-Delgado, Nishino and Sierra [1] (hereafter referred to as DMNS) investigated the matrix product method (MPM) [2], comparing it with the infinite-size density matrix renormalization group (DMRG) [3]. For equivalent basis size, the MPM produces an improved variational energy over that produced by DMRG and, unlike DMRG, produces a translationally-invariant wavefunction. The DMRG results presented were significantly worse than the MPM, caused by a shallow bound state appearing at the join of the two DMRG blocks. They also suggested that the DMRG results can be improved by using an alternate superblock construction $[B] \bullet [B]$ for the last few steps of the calculation.

In this comment, we show that the DMRG results presented by DMNS are in error and the artificial bound state produced by the standard superblock configuration is very small even for $m = 2$ states kept. In addition, we calculate explicitly the energy and wavefunction for the $[B] \bullet [B]$ superblock structure and verify that the energy coincides with that of the MPM, as conjectured in [2].

The matrix product method allows full $SU(2)$ symmetry to be utilized in a natural way, and is relatively easy to implement in a practical calculation. On the other hand, utilizing such non-Abelian symmetries in DMRG appears, at first sight, to be a more difficult problem and it was not until the invention of the interaction-round-a-face DMRG (IRF-DMRG) by Sierra and Nishino [4] that the first breakthrough occurred. Recently, it has been shown that non-Abelian symmetries can be integrated into the DMRG algorithm directly, without the need for a vertex-IRF transformation [5, 6]. This results in several simplifications over the IRF-DMRG algorithm, while in principle the numerical results should be identical for the two methods. Table I shows the results of a re-examination of the spin-1 Heisenberg chain using the non-Abelian method, originally carried out in reference [5]. The results of DMNS for the ground state energy determined by the MPM and the IRF-DMRG are listed as $e^{\text{MP DMNS}}$ and $e^{\text{DMRG DMNS}}$ respectively. Current results using the superblock structure $[B]\bullet[B]$ and $[B]\bullet\bullet[B]$ are listed in columns $e^{1 \text{ site}}$ and $e^{2 \text{ sites}}$ respectively. The DMRG results of DMNS are claimed to use the $[B] \bullet \bullet [B]$ structure, hence the energies in columns $e^{\text{DMRG DMNS}}$ and $e^{2 \text{ sites}}$ should agree exactly. The discrepancy is, we believe, due to a problem with the implementation of the IRF-DMRG algorithm used by DMNS. While there is still a shallow bound state located in the center of the superblock, the effect on the ground state energy is several orders of

TABLE I – *Energy density of the spin 1 Heisenberg chain as a function of number of states kept.* $e^{MP\ DMNS}$ *and* $e^{DMRG\ DMNS}$ *are from reference* [1].

m	$e^{\text{MP DMNS}}$	$e^{\text{DMRG DMNS}}$	$e^{1\text{ site}}$	$e^{2\text{ sites}}$	$1-P_m$
1	−1.333333	−1.333333	−1.3333333	−1.3333333	1.58×10^{-2}
2	−1.399659	−1.369077	−1.3996590	−1.3996237	4.06×10^{-4}
3	−1.401093	−1.392515	−1.4010933	−1.4010886	5.39×10^{-5}
4	−1.401380	−1.401380	−1.4013806	−1.4013798	1.63×10^{-5}
5	−1.401443	−1.401436	−1.4014447	−1.4014430	7.77×10^{-6}
6	−1.401474	−1.401468	−1.4014757	−1.4014756	1.35×10^{-6}

magnitude smaller than reckoned by DMNS. Figure 1 shows the bond energy $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \rangle$ as a function of lattice position for $m = 2$ states kept. For the superblock structure $[B] \bullet [B]$, the bond energy is exactly translationally invariant as predicted by DMNS and is shown here with a solid line. In this case, the bond energy for different values of m (column $e^{1\text{ site}}$ in table I) agrees with that calculated by the matrix product method by DMNS (column $e^{\text{MP DMNS}}$ in table I), verifying the conjecture that the wavefunctions produced by these two algorithms coincide in the thermodynamic limit.

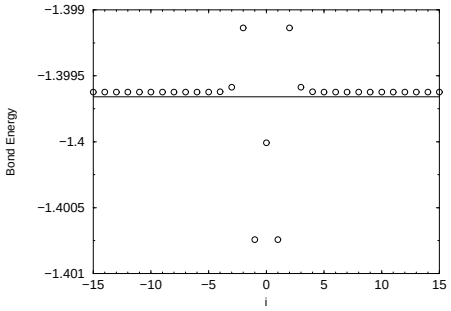

Fig. 1 – Bond energy $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \rangle$ as a function of lattice position for the DMRG wavefunction of the spin 1 Heisenberg chain with $m = 2$.

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